Simulating the Universe at Petascale

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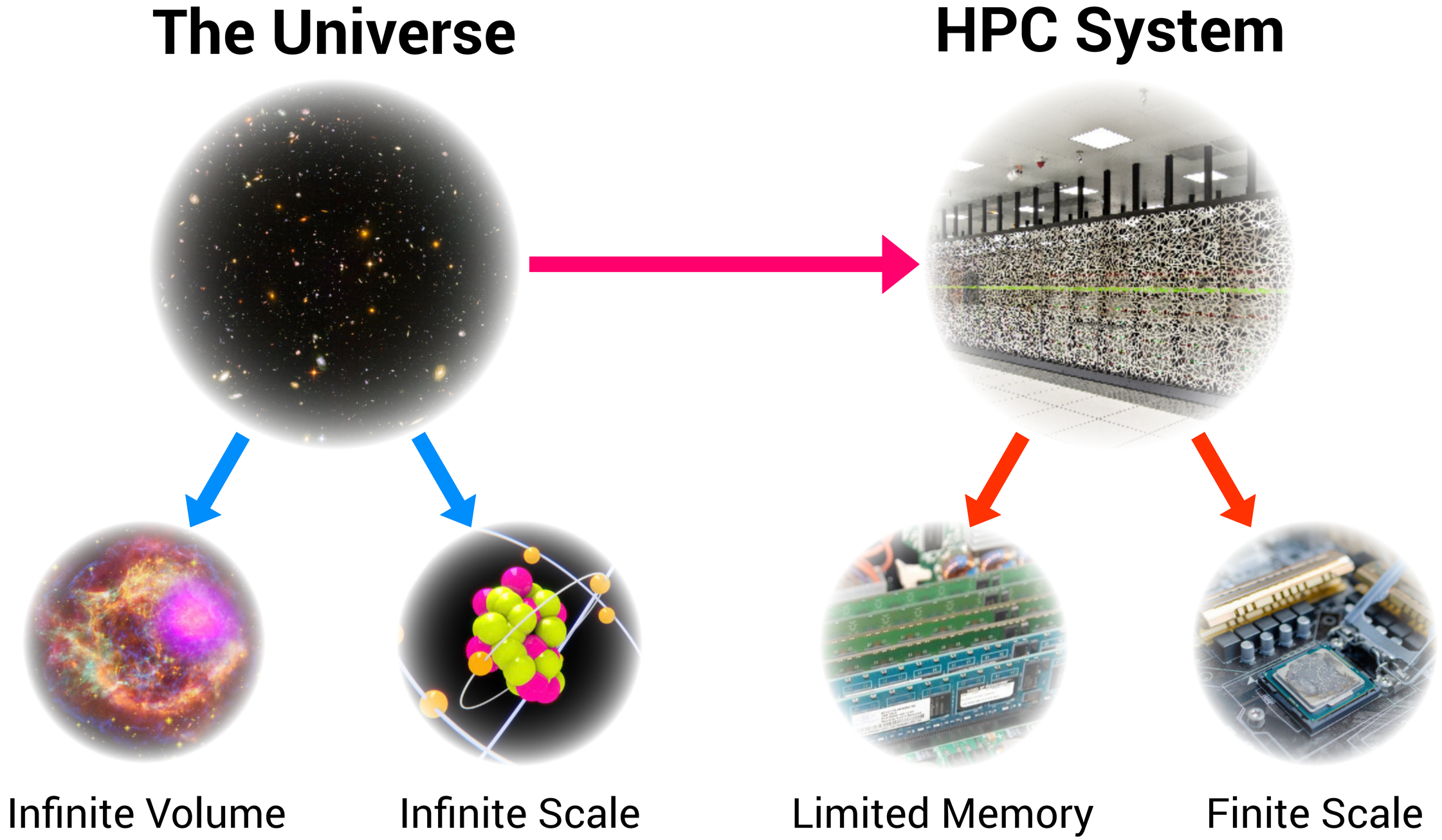
The Universe
HPC System
Infinite Volume
Infinite Scale
Limited Memory
Finite Scale

To what end?

- Astronomers only see a snapshot of the universe
- Impossible to see time-variation
- Linking **properties of galaxies with their dynamical evolution** and environment is then very difficult
- Simulations allow us to do this.

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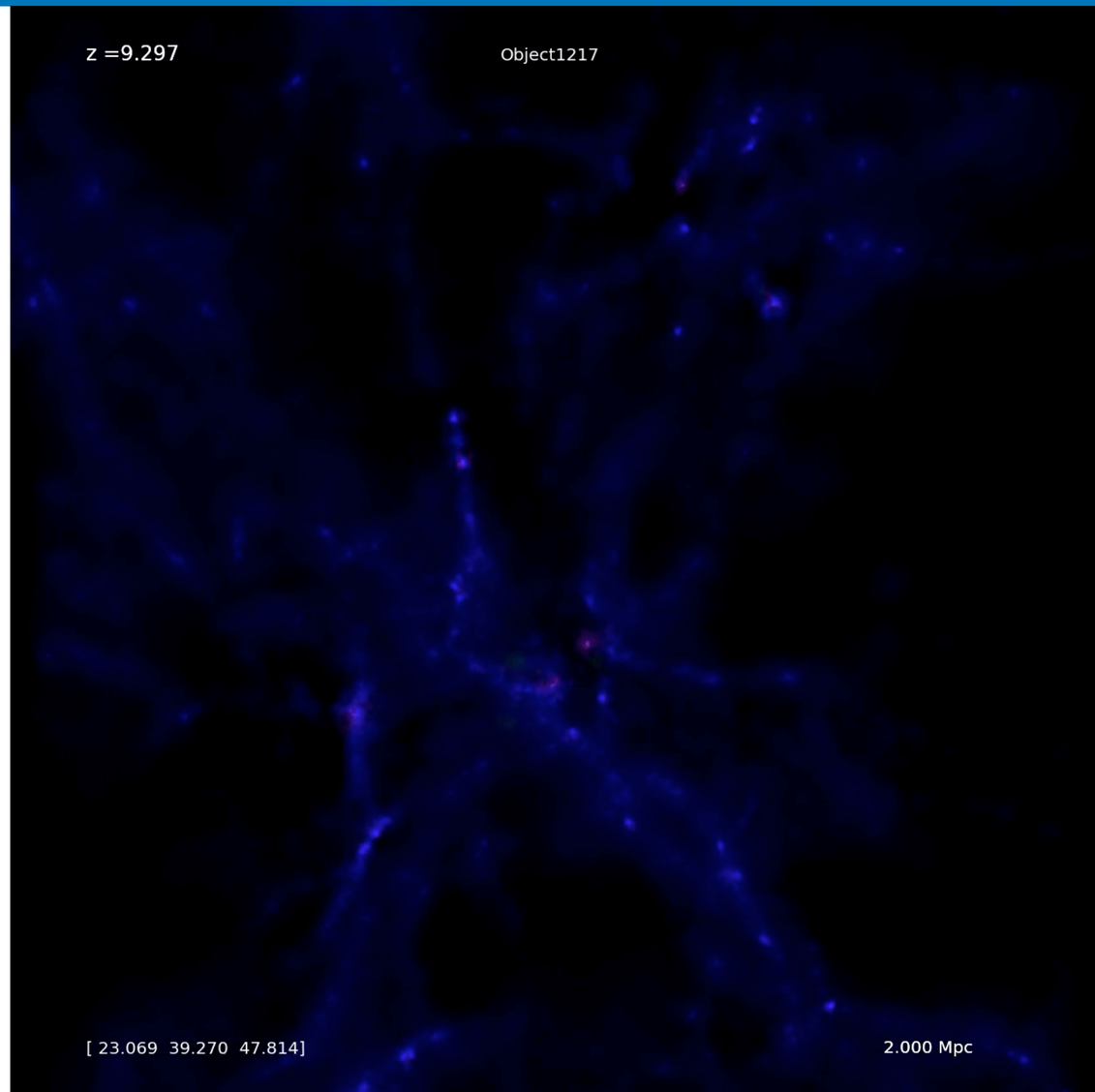
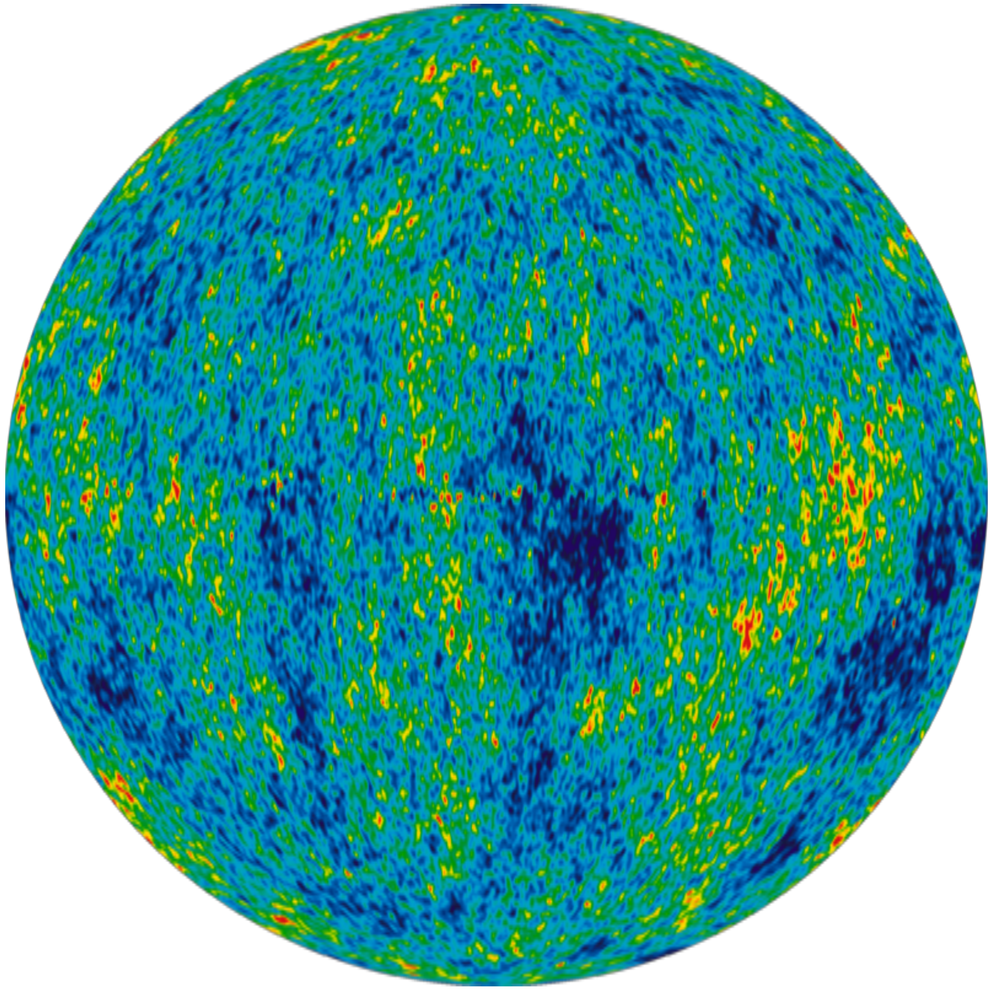


Running a simulation

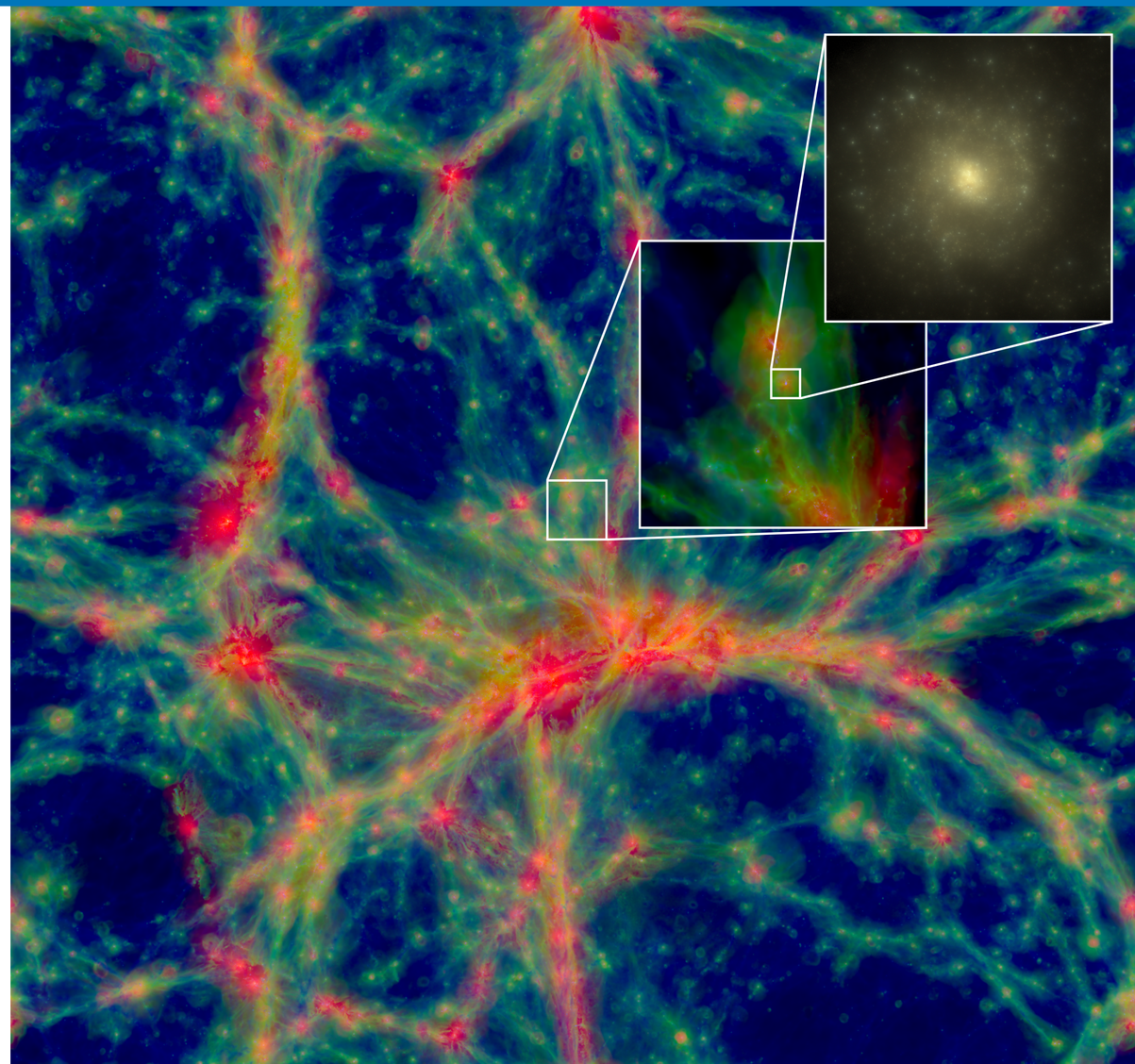
- Take a big bit of Universe (1 billion lightyears on a side)
- Get your **boundary conditions** from the Cosmic Microwave Background (380’000 years after big bang)
- Press play
- …
- Take a look at the galaxies you get



The cosmic microwave background (CMB) as seen by WMAP

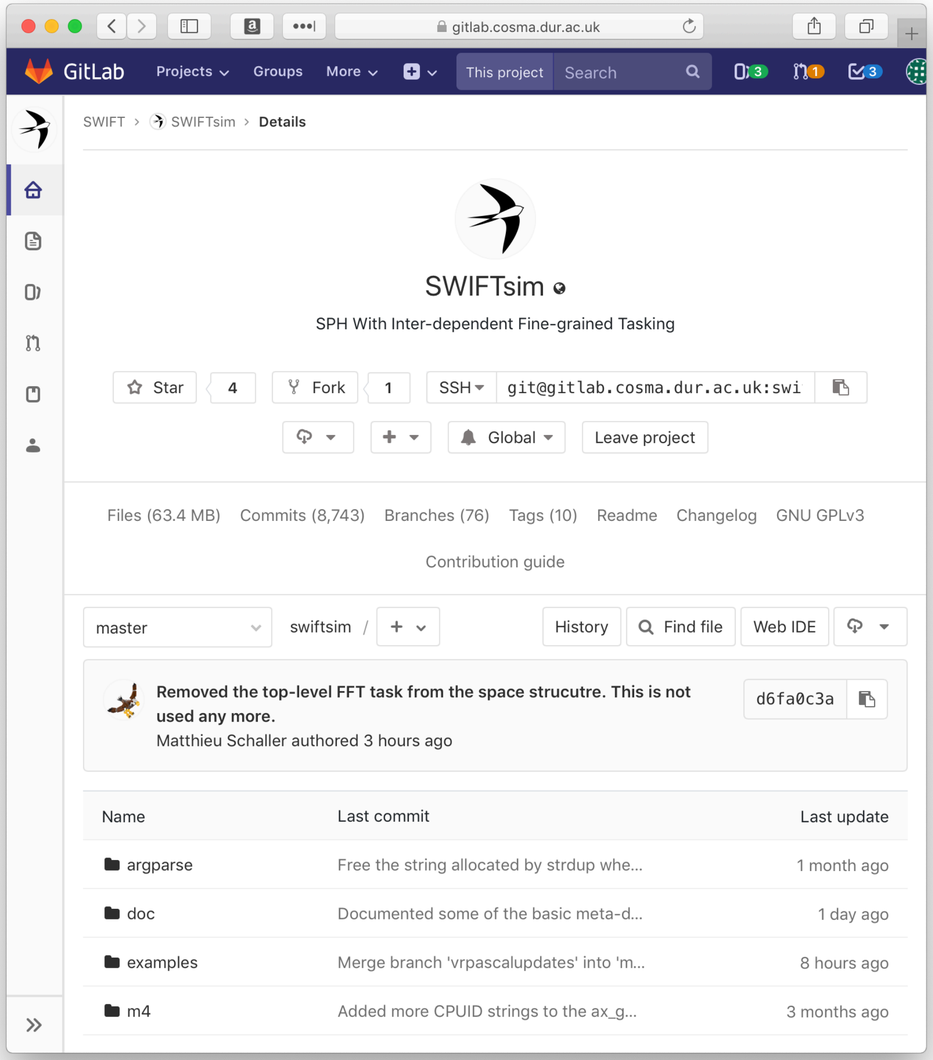
On what scale?

- Our next big run:
- Nearly **100 billion particles**
- 30’000 galaxies with a mass similar to our own Milky Way
- Each galaxy resolved by 10’000 - 100’000 particles



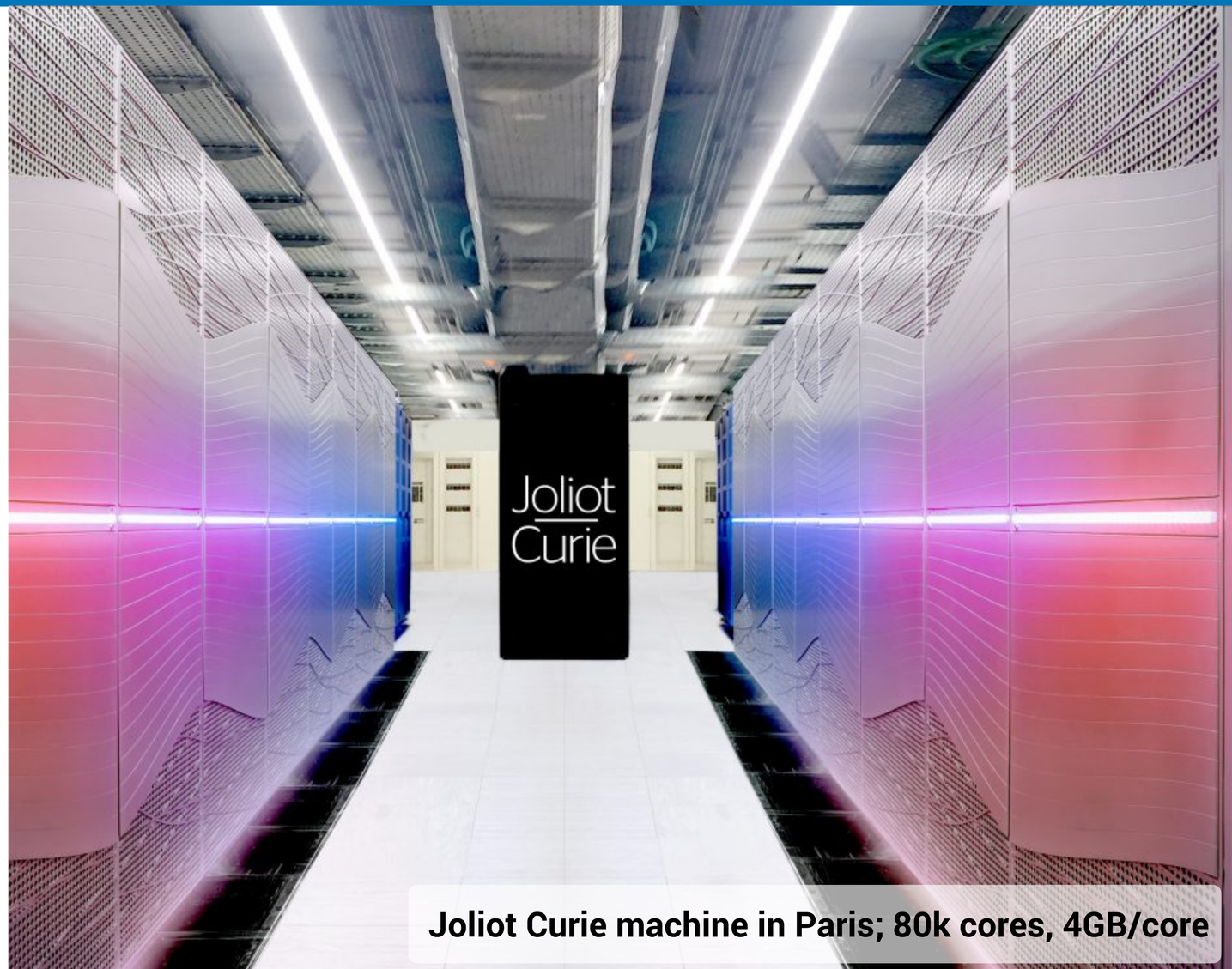
What kind of code?

- 100’000 lines of open-source C99 code
- **Hybrid** (MPI + threads)
- Collaboration between astronomy, computer science, and industry
- Supported by DiRAC



What kind of resources?

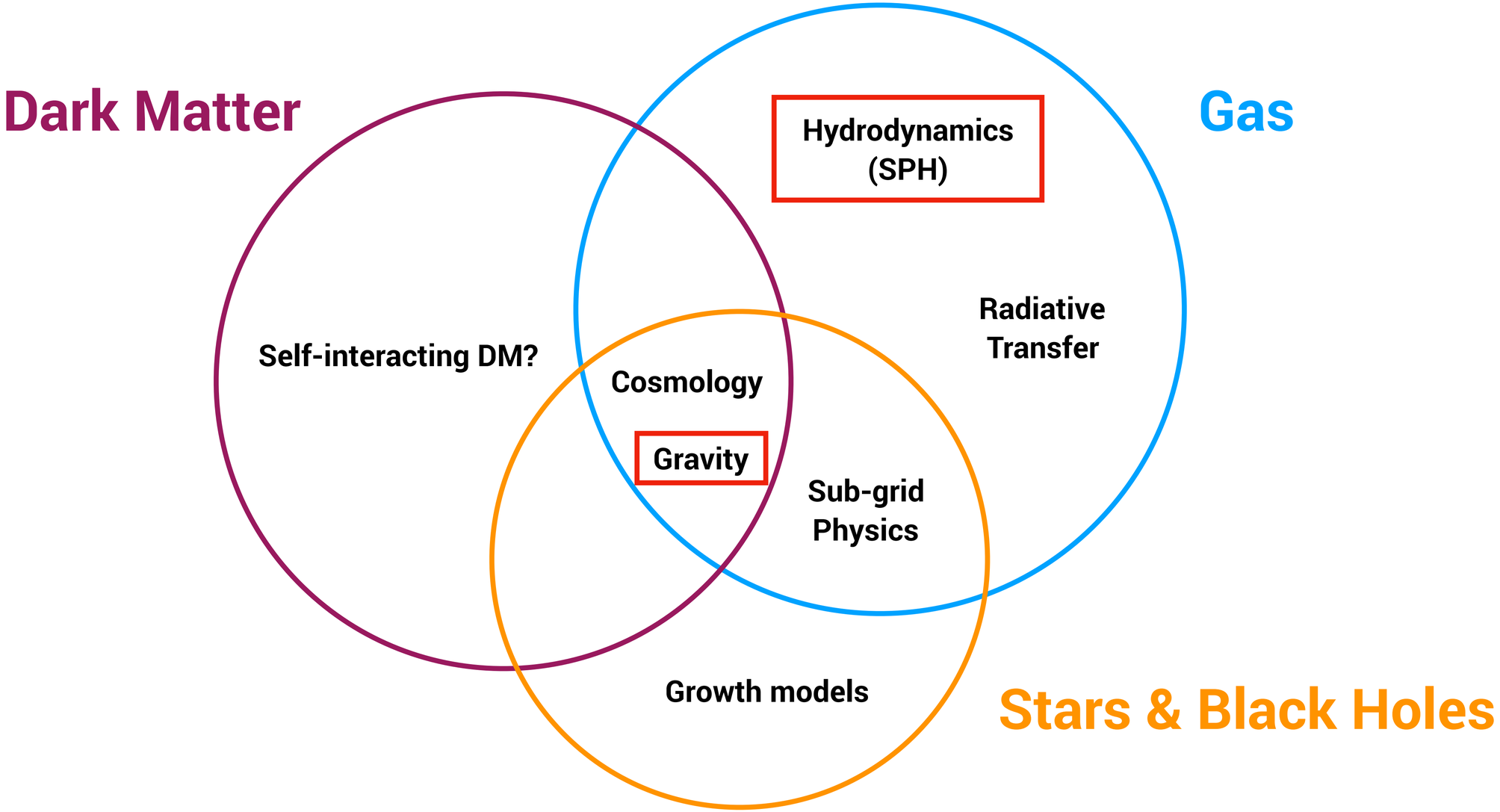
- Need Tier-0 resources
- 10s of millions of core hours
- 10’000s of CPUs
- **~200-300 TB of RAM**
- Snapshots ~4-5 TB each



Joliot Curie machine in Paris; 80k cores, 4GB/core

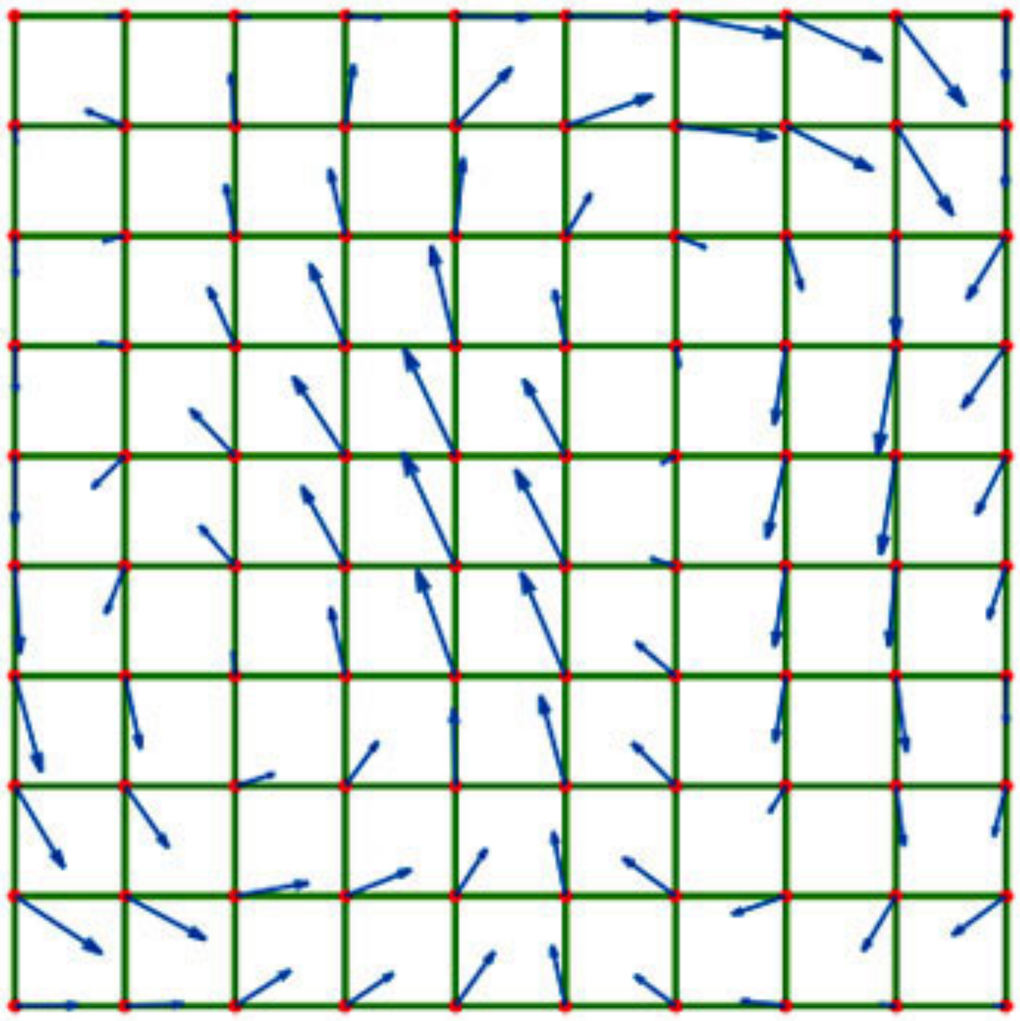
Techniques

What do we need?

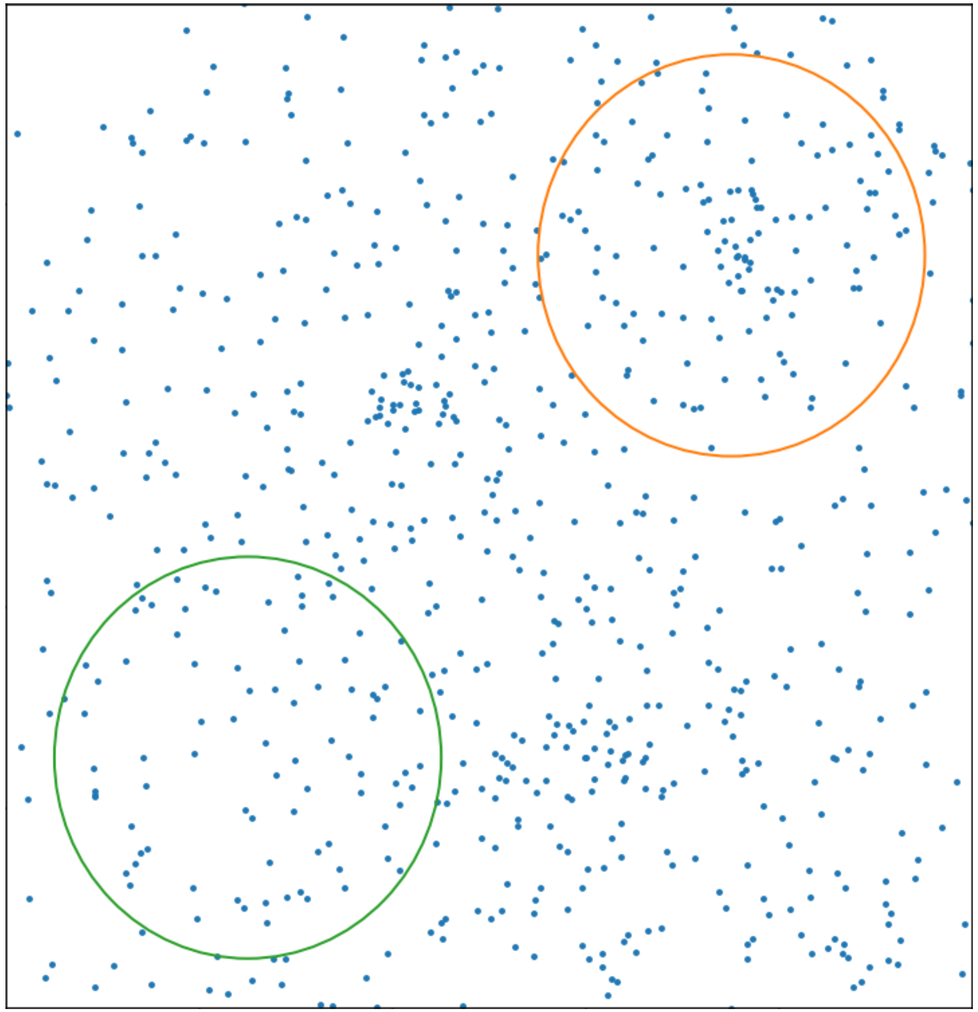


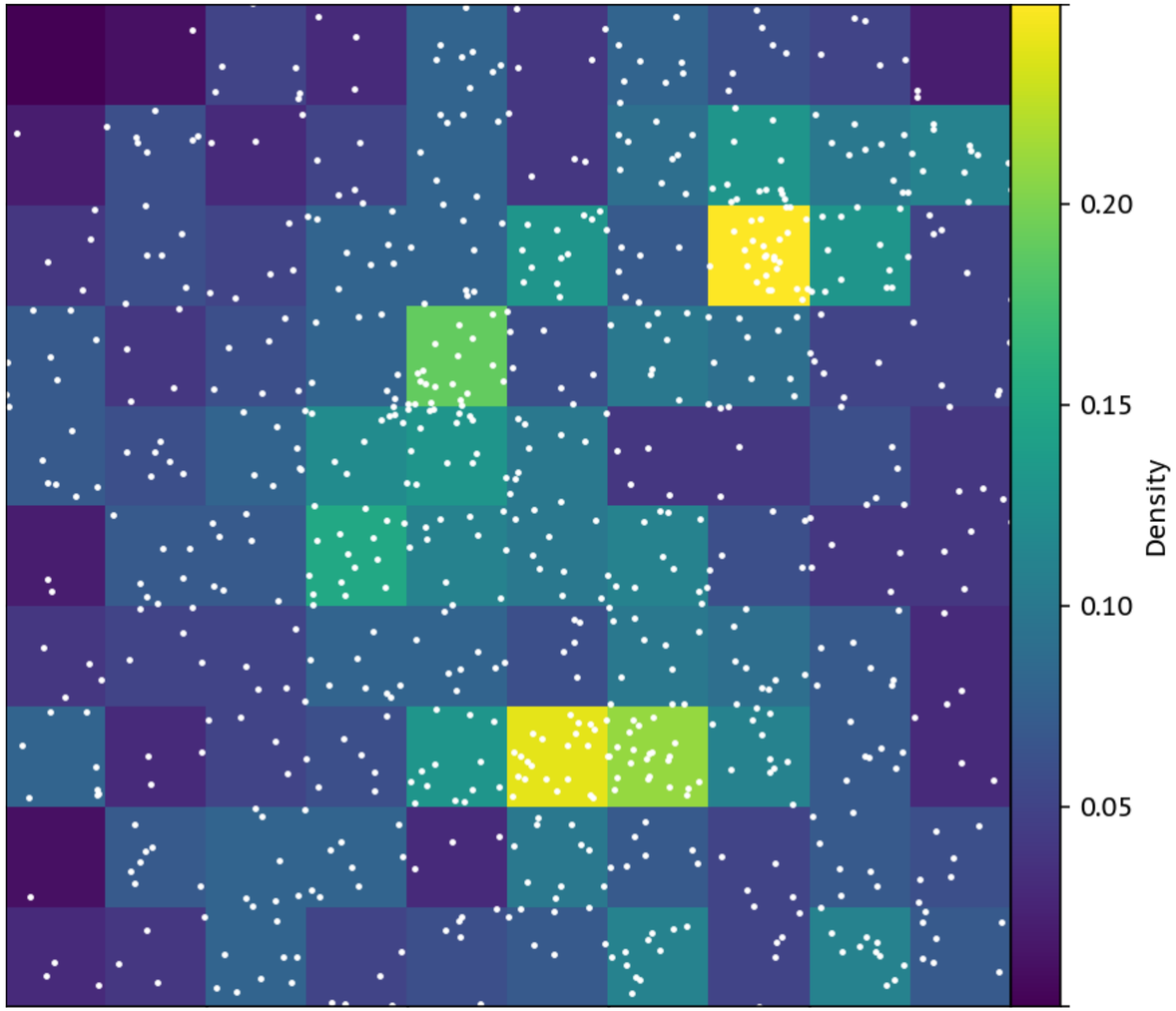
Hydrodynamics

- Typical way to do this: lay down a grid and compute fluid flows between cells
- Several problems:
  - Lack of adaptivity
  - **Cannot track fluid flow over time**
  - Makes gravity difficult



Smoothed Particle Hydrodynamics (SPH)

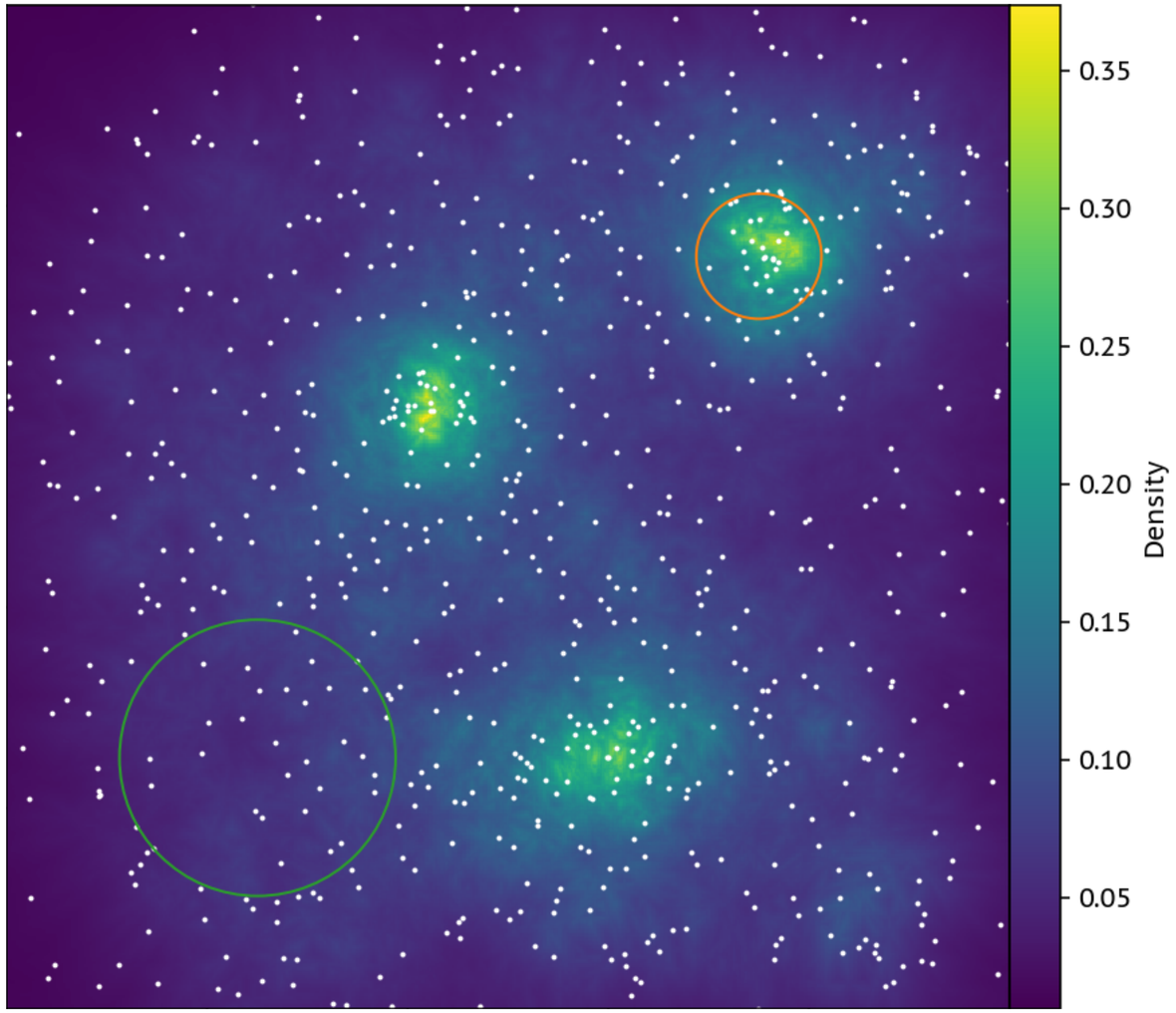




Improving our density estimate

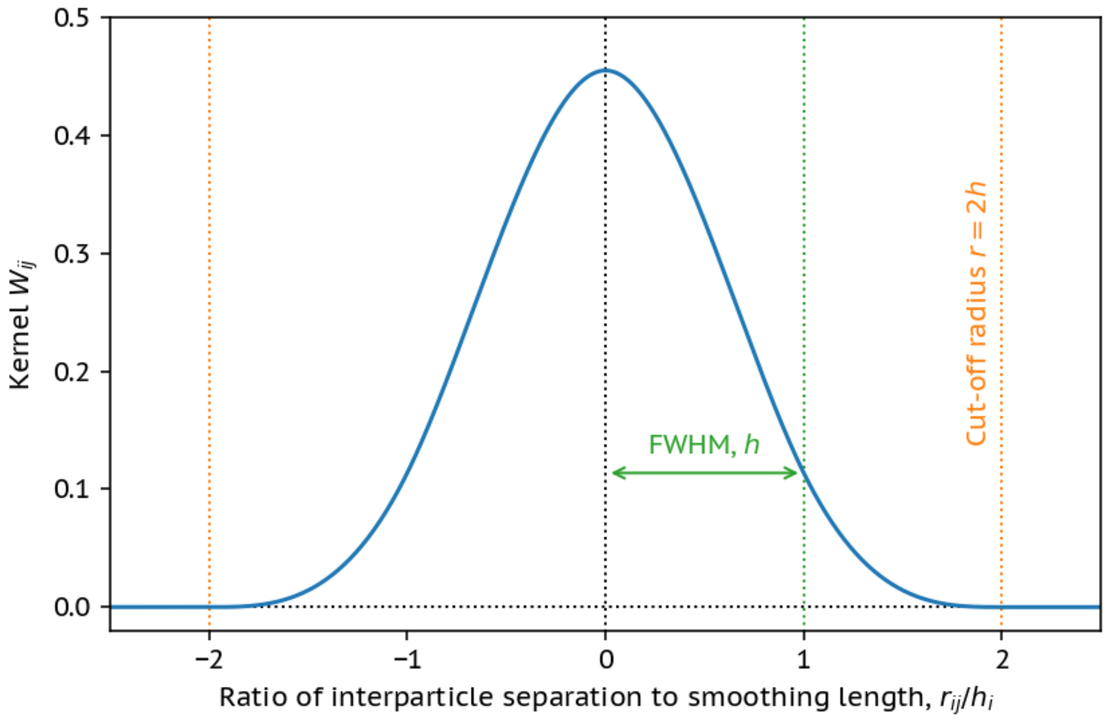
- What if we **change the volume** we consider for each particle?
- Set *R* such that our volume encloses 30 particles.
- Density for each particle is then

$$\rho_i = \frac{30 m_{\mathrm{part}}}{\frac{4}{3}\pi R_i^3}$$



Enter Gaussian filtering?

- We can do better! We **care less about particles that are further away**.
- Weight the contribution from each particle with a “kernel”.
- Size kernel to enclose 30 particles within cut-off radius.

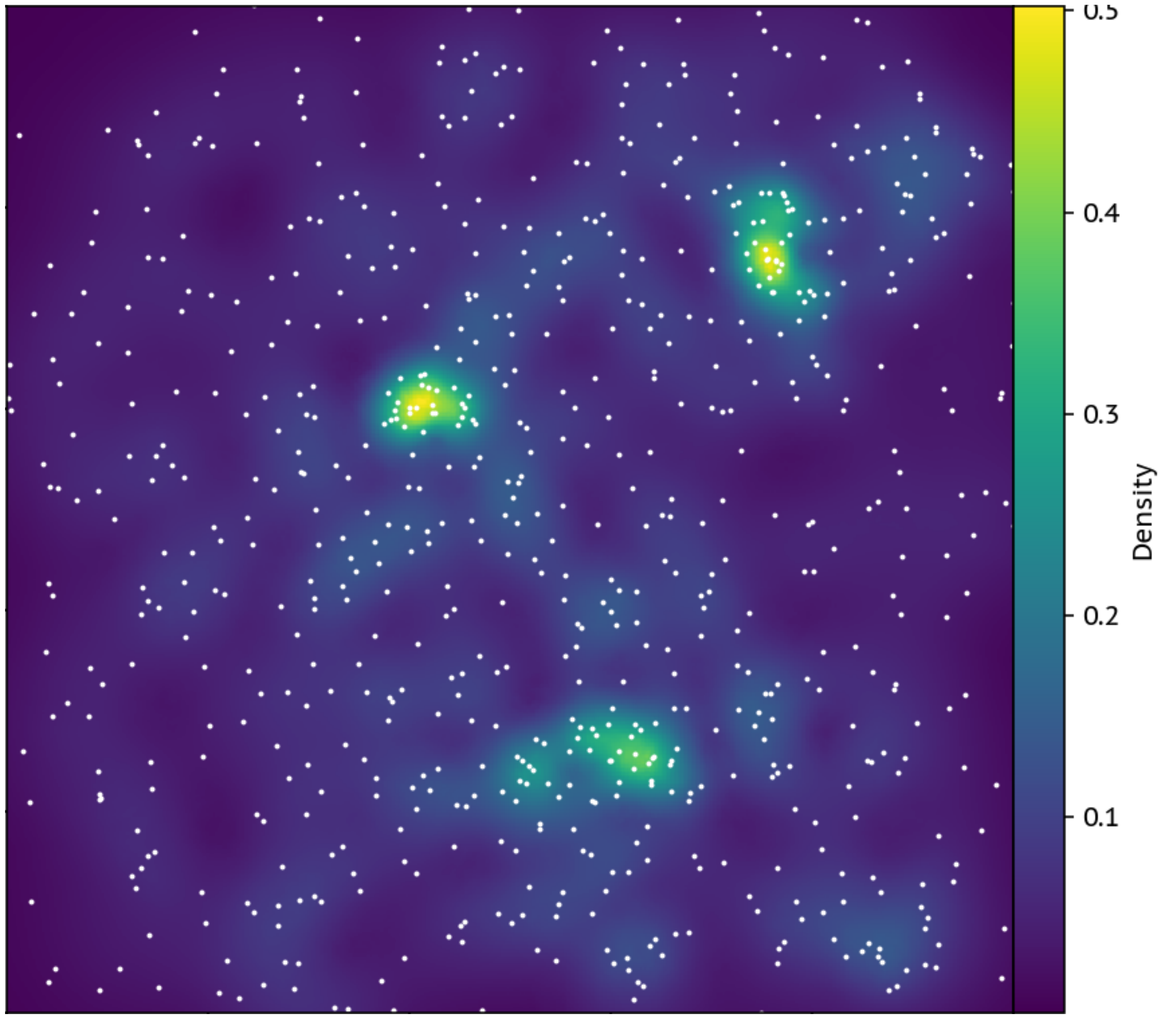


A smooth density estimate

- Density for each particle now given by:

$$\rho_i = \sum_{j=1}^{30} m_{\mathrm{part}} W(r_{ij}, h_i)$$

- Density (+ temperature, tracked by particles) gives **pressure, which gives dynamics**



Adding in the ‘Dynamics’

$$L(q,\dot{q}) = \frac{1}{2}\sum_{i=1}^{N} m_i \dot{r}_i^2 - \sum_{i=1}^{N} m_i u_i,$$

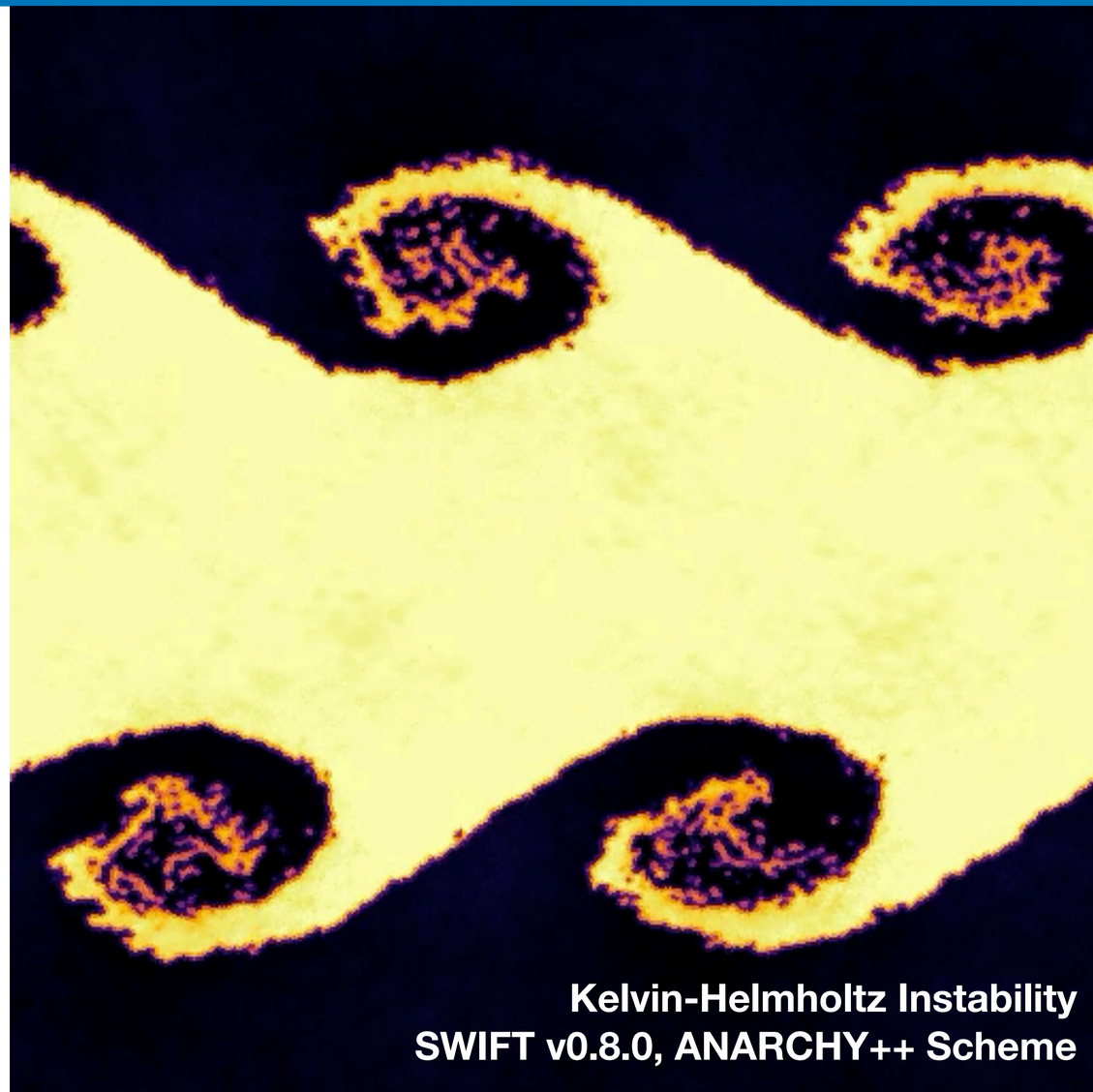
$$\left.\frac{\partial u_i}{\partial q_i}\right|_A = -\frac{P_i}{m_i}\frac{\partial \Delta V_i}{\partial q_i},$$

+

$$\phi_i(\mathbf{q}) = \kappa h_i^{n_d}\frac{1}{\Delta \tilde{V}} - N_{ngb} = 0,$$

$$m_i \frac{\mathrm{d}\mathbf{v}_i}{\mathrm{d}t} = \sum_{j=1}^{N} P_j \nabla_i \Delta \tilde{V}_j \psi_j + P_j \nabla_i \Delta V_j.$$

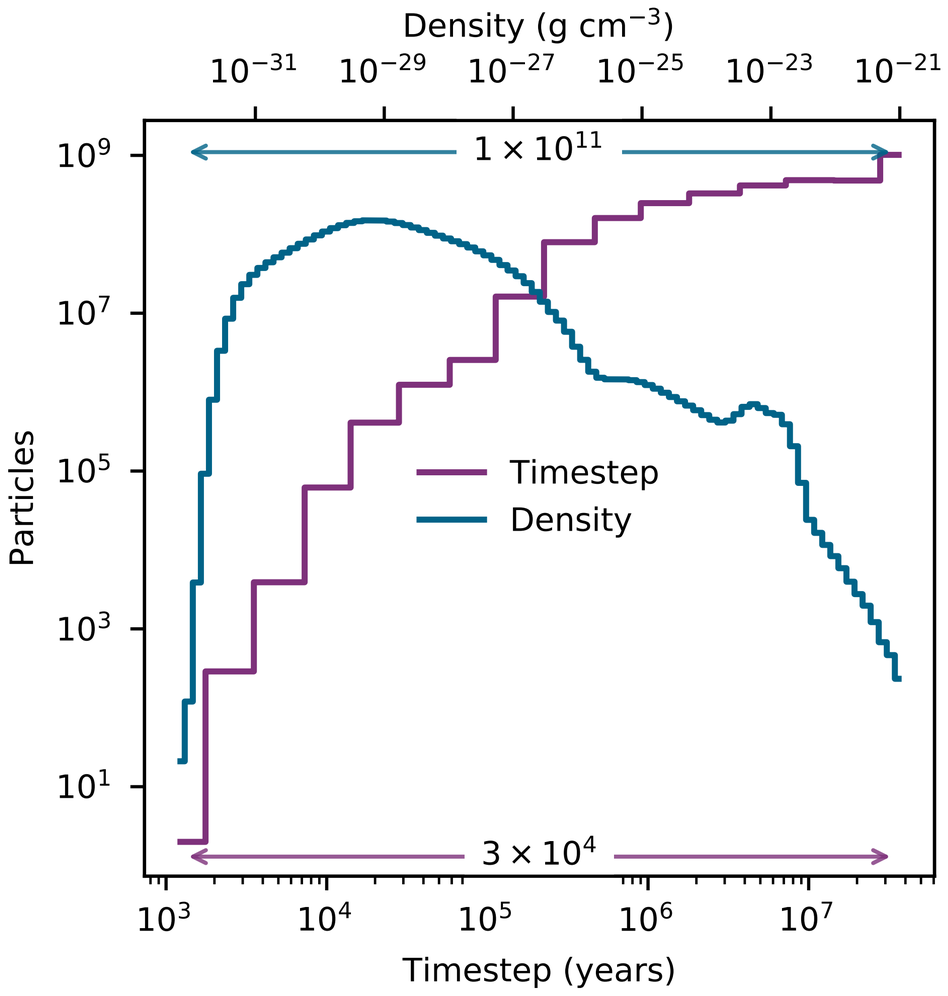
$$\frac{\mathrm{d}\mathbf{v}_i}{\mathrm{d}t} = -\sum_{j=1}^{N} x_i x_j \left[\frac{f_{ij}P_i}{y_i^2}\nabla_i W_{ij}(h_i) + \frac{f_{ji}P_j}{y_j^2}\nabla_i W_{ji}(h_j)\right]$$



Simulating at Scale

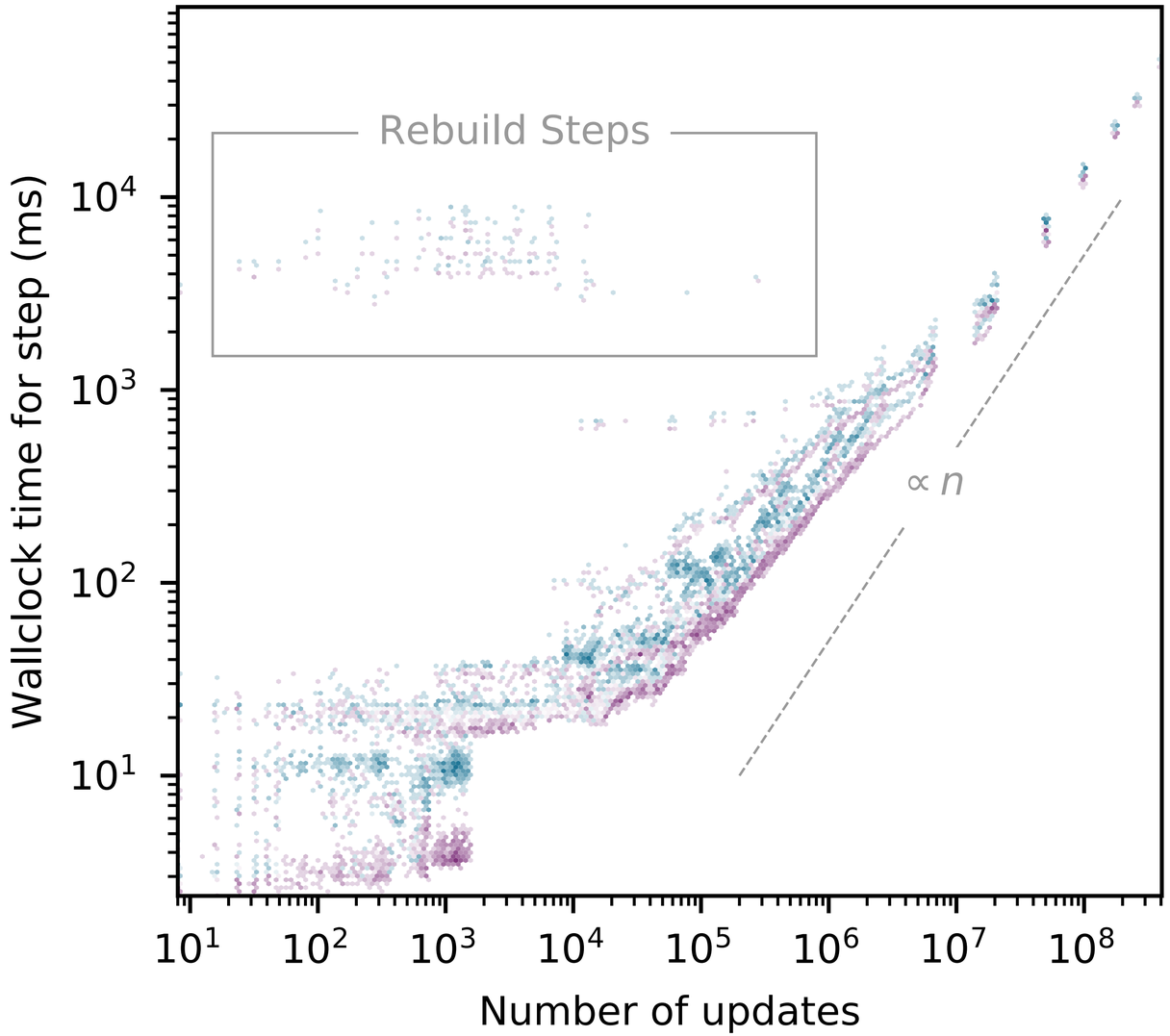
Why is hydrodynamics so challenging?

- We must use a multiple time-stepping scheme; each particle has it's own *dt*
- This is required because of the **huge range in density** in these simulations (voids through to the cores of galaxies)
- Not using such a scheme causes a ~**100-1000x** degradation in performance.



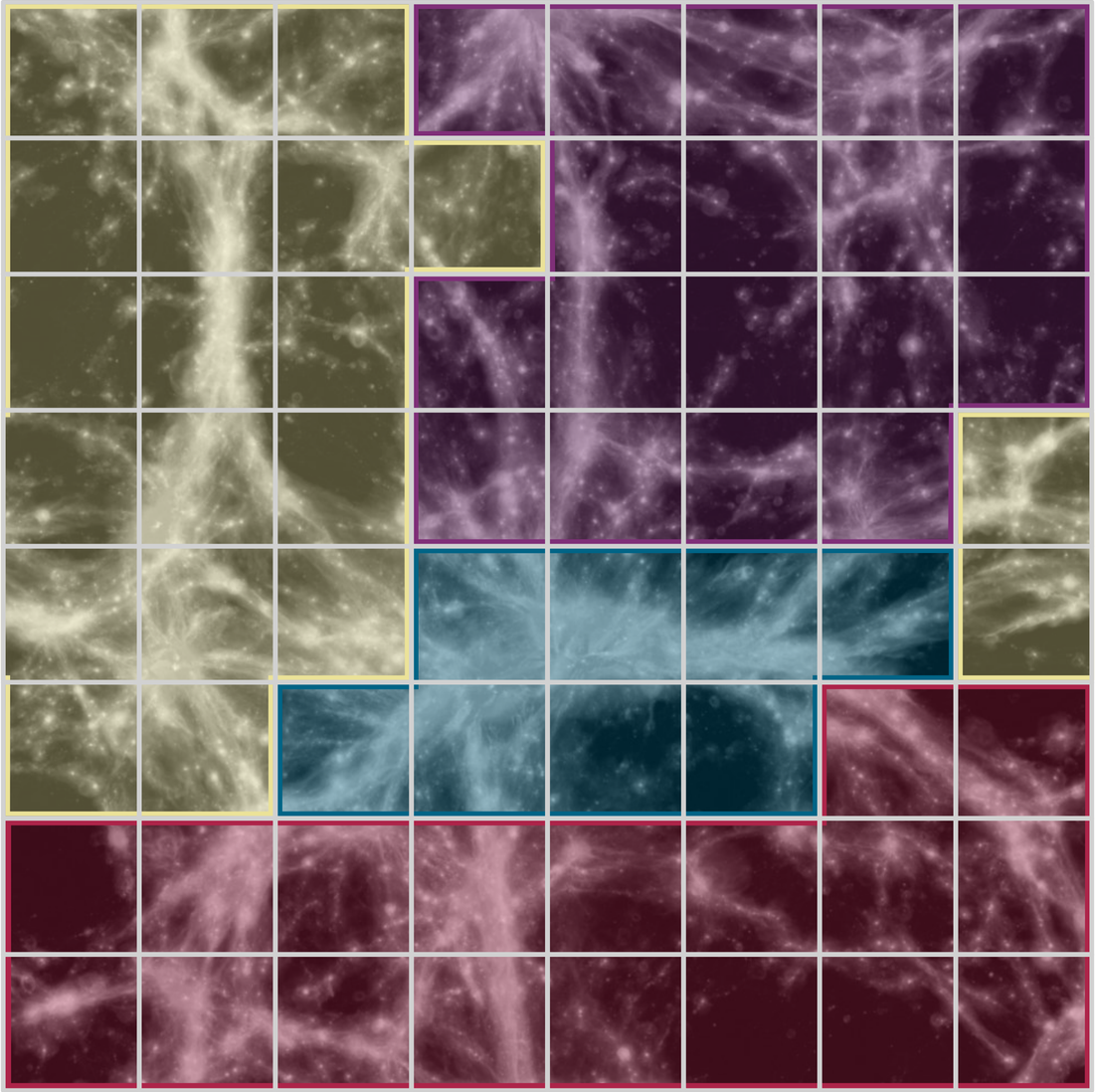
How does this cause a problem?

- Each dot represents a step in the simulation
- “easy” to scale large steps
- Small steps very difficult - **handful of particles** (out of 200TB worth of ram full) **active**
- Impossible to load balance



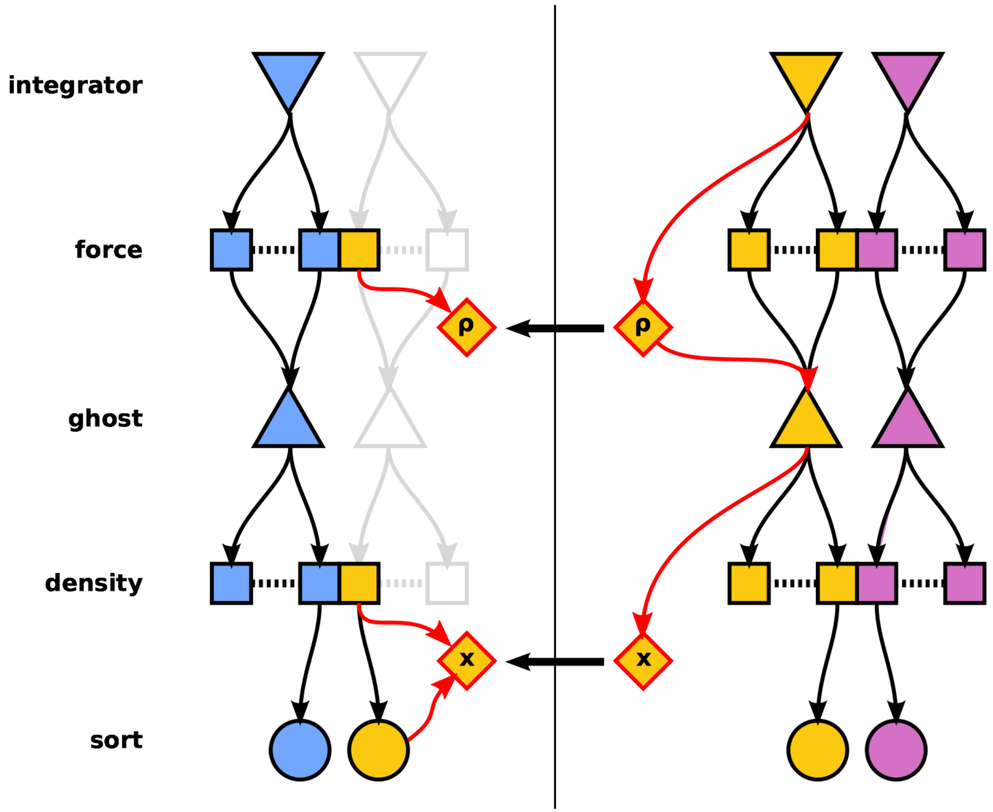
Damage control

- Ensure there is **no MPI** (communication) **in the short steps**
- Do this by using a strategy that places the particles for a galaxy at the “center” of a node
- This ensures short steps are as short as possible; latency kills you.



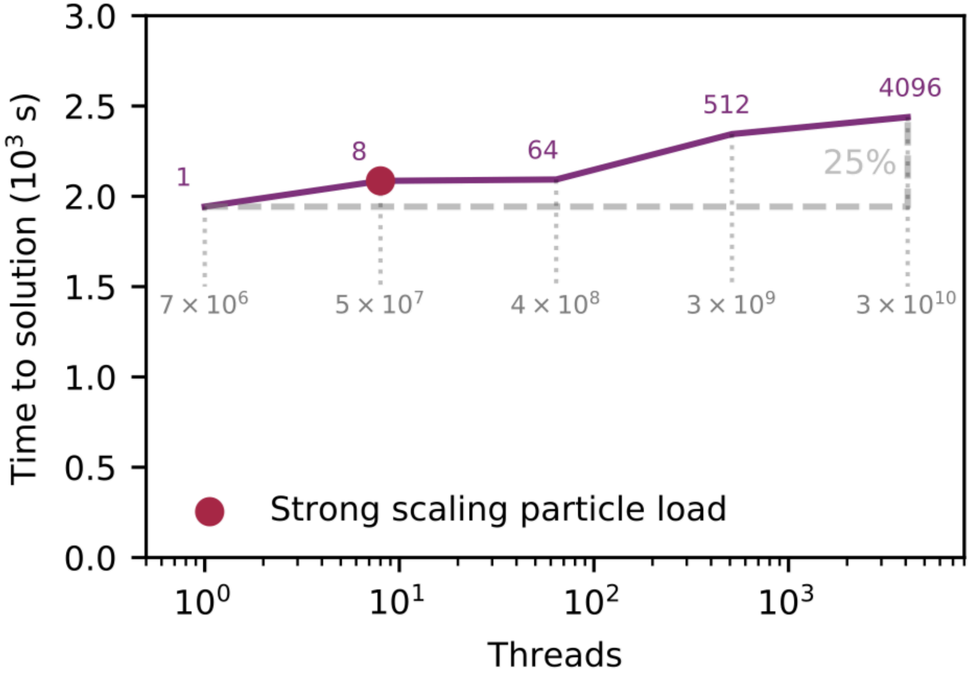
Other incremental improvements

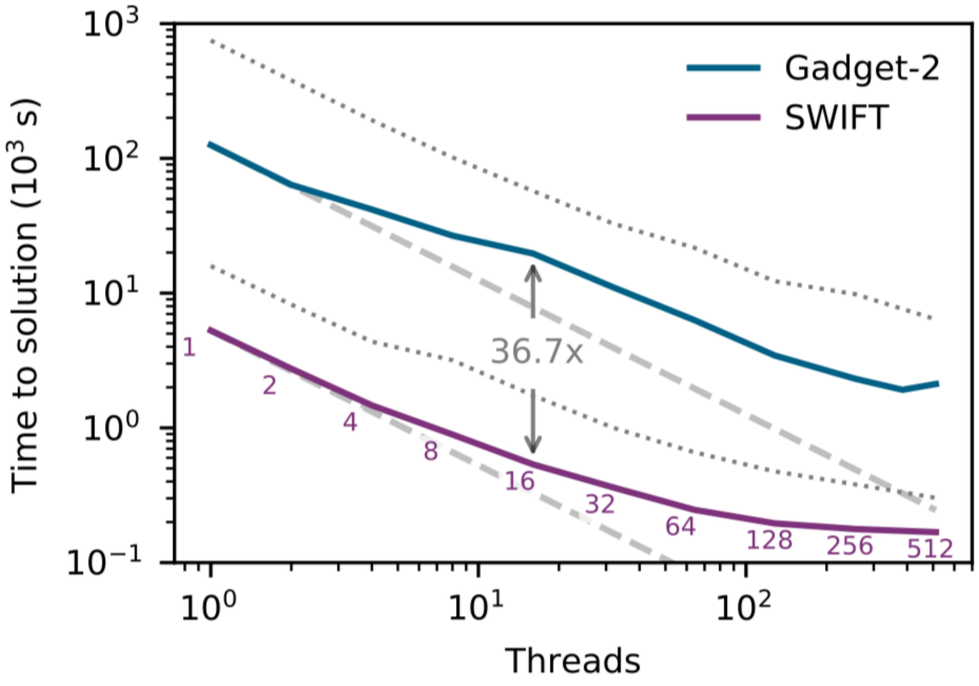
- Hand-written AVX-512 kernels for particle interactions (~3-4x speedup)
- Smart algorithms for finding neighbours (~5x speedup)
- Asynchronous communications & better load balancing (~2x speedup)



Does this actually work?

- Yes!
- Normally weak-scaling such a problem is incredibly difficult.
- Larger simulations -> more dense regions -> larger time-step hierarchy.

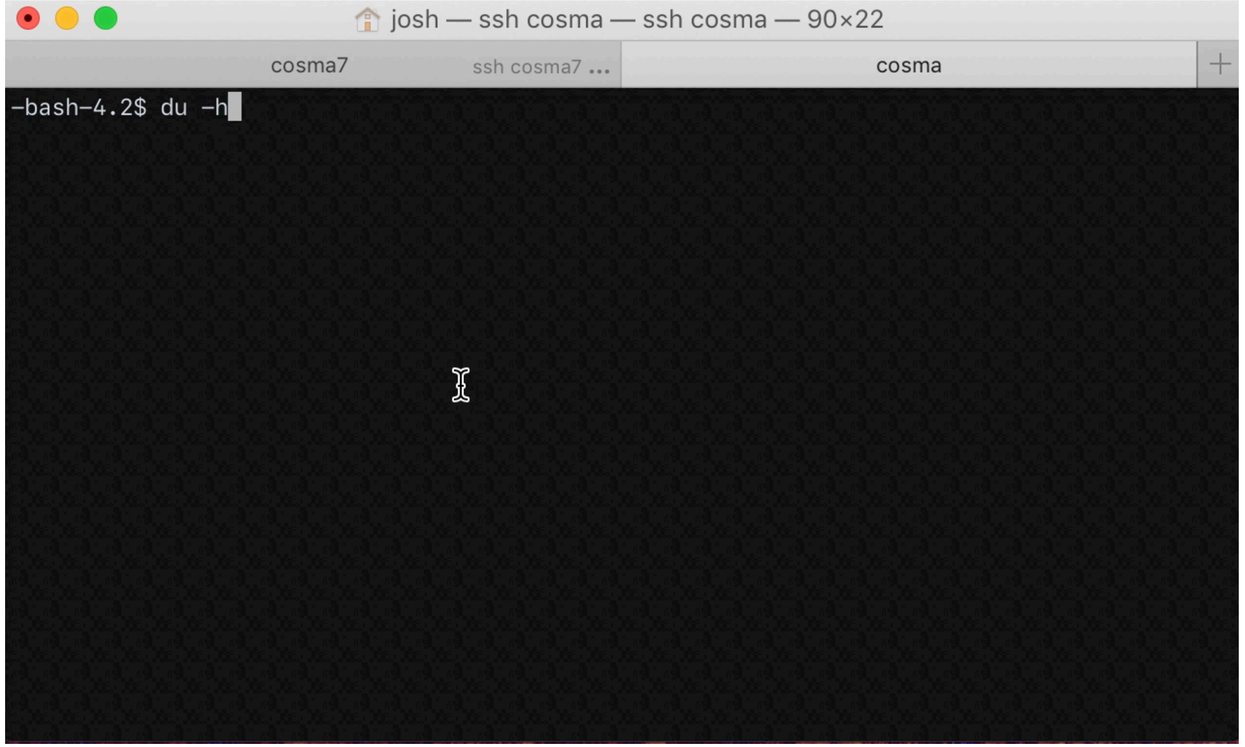




Dealing with Data

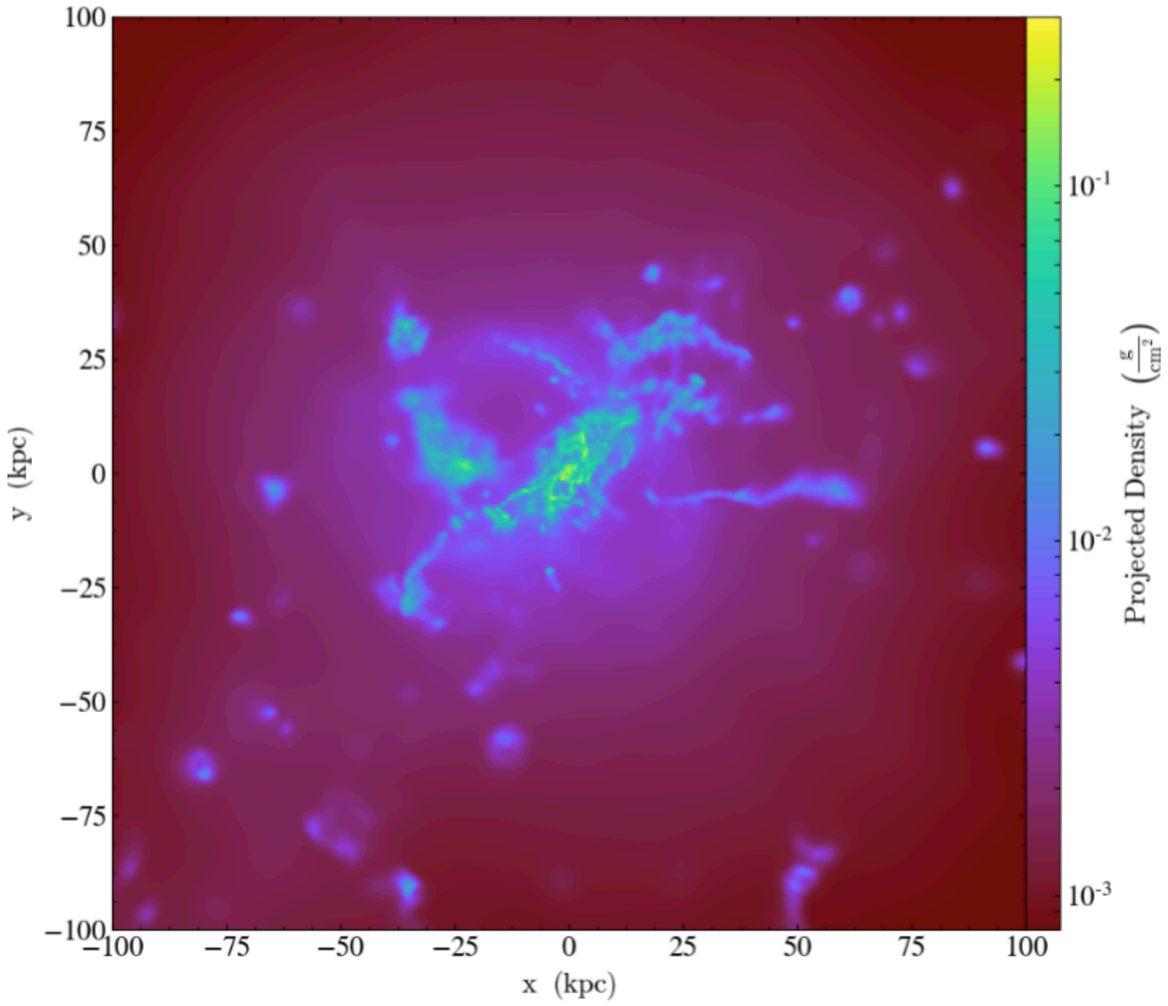
Data sizes

- A full run of our production simulation will produce **3 PB** of data.
- This is untenable to store!
- Need on-the-fly analysis



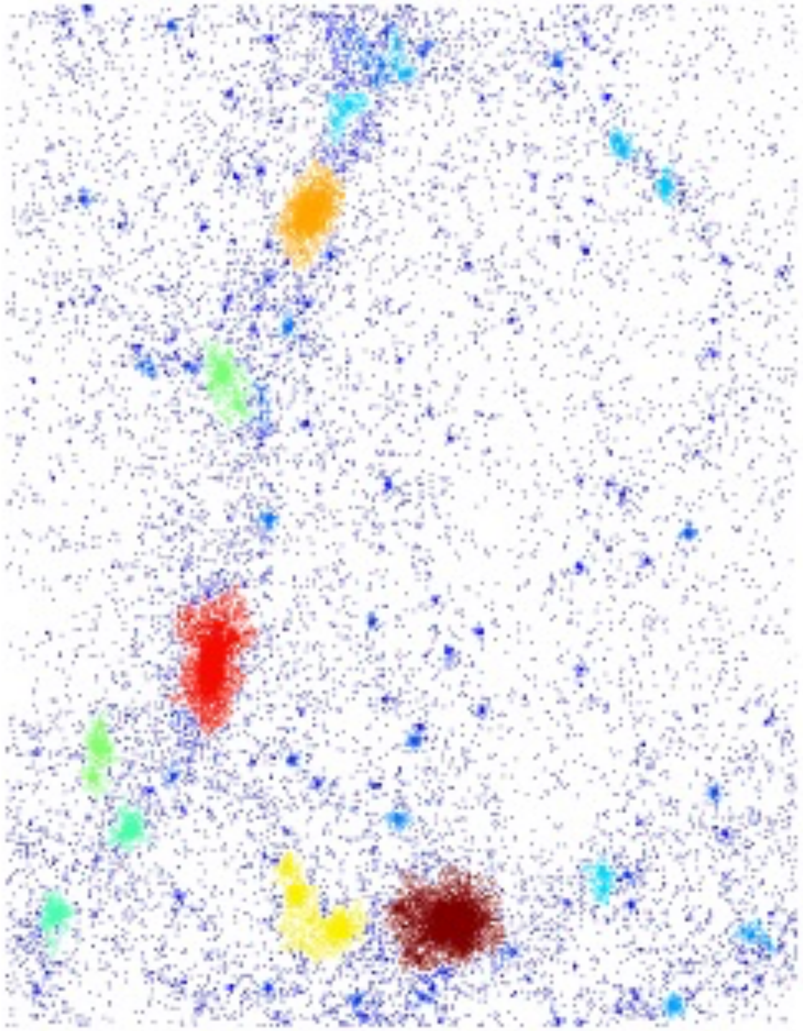
Choices of tools

- Unfortunately, `pandas.df("cosmological_simulation")` doesn't quite cut it
- Pandas has a 5-10x memory overhead and cannot deal well with partial reads
- We have **custom-built tools** (e.g. yt & unyt NUMFOCUS projects)



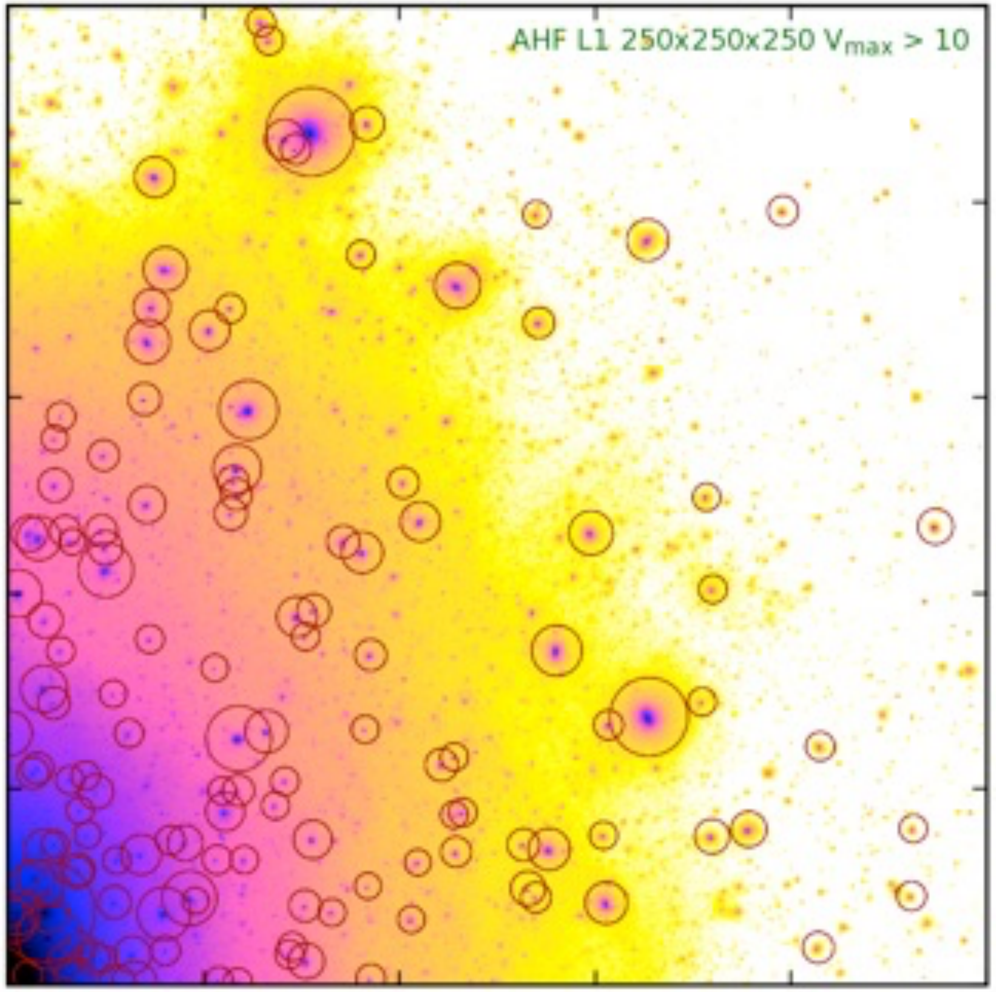
How do we find structures?

- We use a 6D friends-of-friends finder (6D FoF)
- This structure finder explicitly does **not require all particles to be in groups**
- Also run an iterative *substructure* search



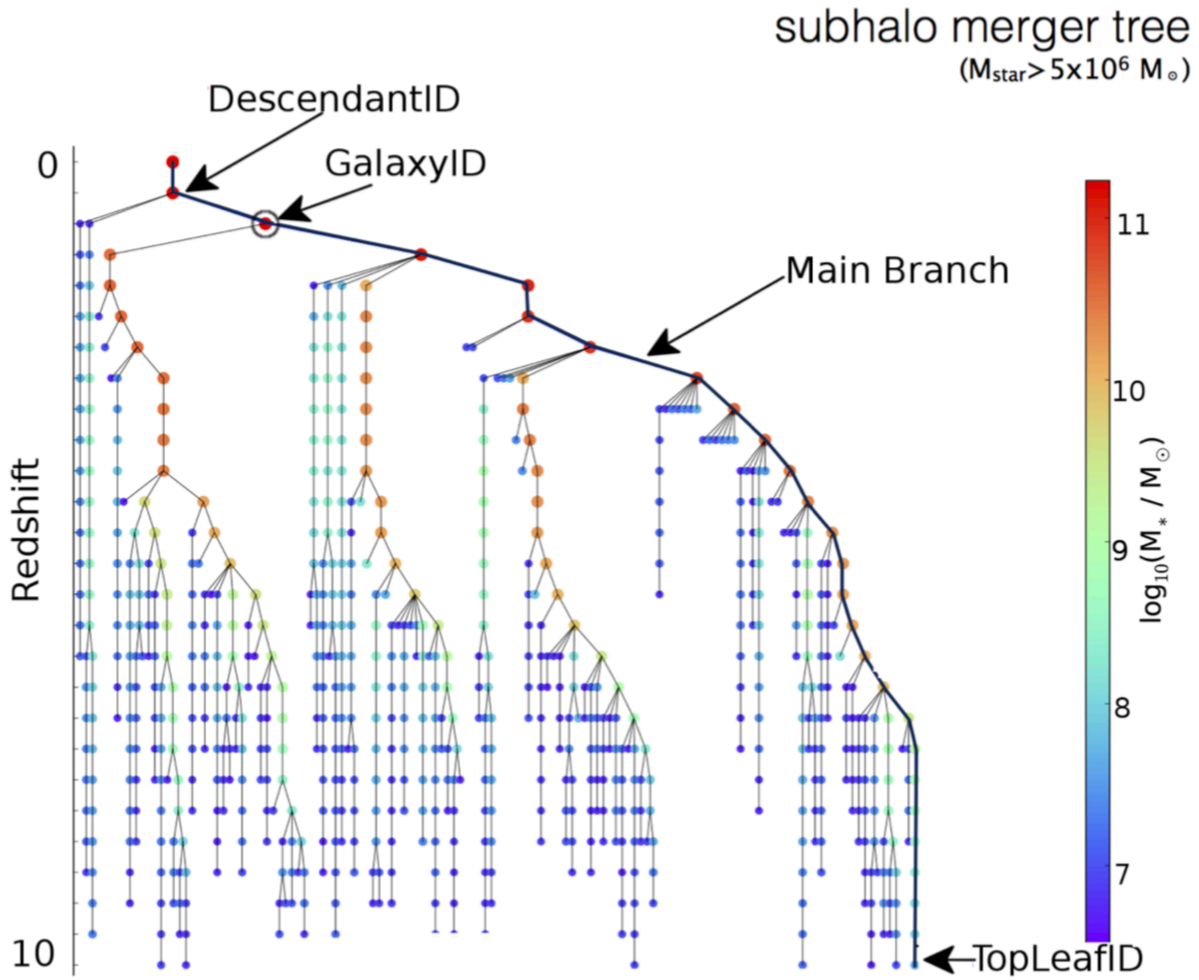
Collecting Metadata

- We run **structure finders on-the-fly** as the simulation is running
- This metadata is saved at higher frequency than snapshots
- Allows us to extract **bound structures from snapshots instantly** (hdf5 is our lord and saviour)



On-the-fly Analysis

- Structure finder also computes galaxy *properties* at higher resolution than snapshots
- Need to link galaxy data together between snapshots
- Tools like tangos help us further process this data (built on sqlalchemy)



Takeaways

- (Hopefully): cosmological simulations are cool!
- Small gains add up; keep making iterative improvements!
- Running on-the-fly analysis is hugely important
- Metadata saves the day (again)
- Some cool tools: yt, unyt, friends-of-friends for clustering

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